On the Absence of Spurious Eigenstates in an Iterative Algorithm Proposed By Waxman

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Abstract

We discuss a remarkable property of an iterative algorithm for eigenvalue problems recently advanced by Waxman that constitutes a clear advantage over other iterative procedures. In quantum mechanics, as well as in other fields, it is often necessary to deal with operators exhibiting both a continuum and a discrete spectrum. For this kind of operators, the problem of identifying spurious eigenpairs which appear in iterative algorithms like the Lanczos algorithm does not occur in the algorithm proposed by Waxman.

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The Hamiltonian operator which describes a quantum mechanical system generally possesses both a continuum as well as a discrete spectrum. A similar situation also occurs in other fields, such as theoretical population genetics [1]. In many cases one is only interested in a few of the lower-lying bound states of the system. When only bound states are present iterative algorithms such as the Lanczos algorithm [2] yield good approximations to the lower-lying eignstates with good convergence properties [3, 4, 5, 6]. On the other hand, the presence of the continuum leads to complications which can be circumvented but not without introducing spurious eigensolutions that need to be identified and eliminated [7]. Such spurious eigensolutions, however, do not occur in an algorihthm recently proposed by Waxman[8]. We compare the two algorithms and demonstrate this behaviour in a simple numerical example.

The presence of the continuum leads to complications in the Lanczos algorithm[2]. Finding a suitable start vector is by no means trivial[9] since the Lanczos algorithm can only be applied to states which are normalizable in the $\mathcal{L}^2$ sense. For those operators which possess a continuum as well as a point spectrum, the space spanned by the bound state eigenfunctions is by itself certainly not complete and a suitable start vector should be composed only of components in the subspace spanned by the bound state eigenvectors. Usually the start vector is chosen from a complete set of analytic $\mathcal{L}^2$ functions which define a space $\mathcal{F}$. This space is in most cases not necessarily of the same dimension as the subspace spanned by the exact eigenvectors. On the other hand, if the Lanczos algorithm is applied with this choice for the start vector, the eigenpairs obtained will correspond to those of the operator $\hat{H}$ projected onto $\mathcal{F}$. A subset of these eigenstates must correspond to the exact eigenpairs of the unprojected Hamiltonian operator since the exact eigenstates can be expanded in terms of the complete set of states which span $\mathcal{F}$. The exact bound states can be identified and separated from the spurious bound states in the following manner[7]. After each iteration, for each of the converging eigenpairs $(e_{l\beta}, |e_{l\beta}\rangle)$, $\Delta_{l\beta} = |e^2_{l\beta} - < e_{l\beta}|\hat{H}^2|e_{l\beta} > |$ (where l is the iteration number) is calculated and a determination is made as to whether Δ is converging toward zero or not. For the exact bound states of $\hat{H}$, Δ must be identically zero while the other spurious eigenstates states of the projected operator should converge to some non-zero positive value. Provided sufficient iterations are performed, it is possible, in this manner to identify uniquely the approximate eigenpairs which ultimately will converge to the exact bound states.

In the present note we wish to point out that this difficulty is avoided in a recently proposed iterative algorithm for determining the bound state eigenpairs of linear differential operators such as the Schrödinger Hamiltonian[8]. This algorithm has many advantages not the least of which is its simplicity and an excellent convergence rate. The eigenpairs are determined as functions of the strength of the potential in the following manner. For simplicity consider a one-dimensional eigenvalue equation[8]

$$[-\partial_x^2 - \lambda V(x)]u(x) = -\epsilon u(x) \tag{1}$$

$$\lim_{|x|->\infty} u(x) = 0 \tag{2}$$

where $\partial_x = \frac{\partial}{\partial_x}$; $\lambda > 0$ is the strength parameter of the attractive potential (λV(x) < 0 and V(x)$\rightarrow 0$ as $|x| \rightarrow \infty$) and the energy eigenvalue, $-\epsilon$ (with $\epsilon > 0$), is negative and corresponds to a bound state. Using Green's method a solution to eq(1) is given by

$$u(x) = \lambda \int_{-\infty}^{\infty} G_\epsilon(x - x')V(x')u(x')dx' \tag{3}$$

where the Green's function $G_\epsilon(x)$ satisfies

$$[-\partial_x^2 + \epsilon]G_\epsilon(x) = \delta(x) \tag{4}$$

$$\lim_{|x|->\infty} G_\epsilon(x) = 0. \tag{5}$$

Normalizing u(x) at an arbitrary x_{ref}

$$u(x_{ref}) = 1 \tag{6}$$

allows λ to be written as (see eq(3))

$$\lambda = \frac{1}{\int G_\epsilon(x')v(x')u(x')dx'} \tag{7}$$

which can then be used to eliminate λ from eq(3)

$$u(x) = \frac{\int_{-\infty}^{\infty} G_\epsilon(x - x')V(x')u(x')dx'}{\int G_\epsilon(x')v(x')u(x')dx'}. \tag{8}$$

Using equations (7) and (8), λ can be determined as a function of ϵ in the following manner. For a particular choice of ϵ eq(8) can be iterated

$$u_{n+1}(x) = \frac{\int_{-\infty}^{\infty} G_\epsilon(x - x')V(x')u_n(x')dx'}{\int G_\epsilon(x')v(x')u_n(x')dx'} \tag{9}$$

until it converges and λ can then be determined from eq(7). Repeating for different values of ϵ yields a set of different values of the potential strength λ. When enough points have been determined, a simple interpolation procedure yields the dependence of ϵ on λ. Note that no diagonalization is required. In spite of the necessity of interpolating, the rapid convergence of the numerical solution of eq(9) makes the present algorithm extremely viable. Furthermore, a proof of coverconvergence has been given and the algorithm can be extended for the calculation of excited states[8].

In order to demonstrate that spurious solutions do not occur in the aforementioned algorithm we have performed the following simple calculation. An inverse Gaussian potential

$$V(x) = e^{\frac{-x^2}{2}}$$

with half width of $2\sqrt{(2ln(2))}$ has been constructed which does not support any excited bound states. The Lanczos algorithm has been used to determine the eigenstates of the corresponding Hamiltonian operator in one dimension using

$$\phi_1(x) = \langle x|1\rangle = (\frac{2}{\pi})^{1/4} e^{-x^2}$$

as the normalized start vector. After 18 iterations the Lanczos algorithm yielded the ground state at $e_{18\ 1}$ = -0.475917 plus a spurious state at $e_{18\ 2}$ = 0.529612. In the case of the ground state $\Delta_{18\ 1}$ = 0.0218906 while $\Delta_{18\ 2}$ = 2.09673 clearly indicating that the excited state is spurious. The Waxman algorithm, using $u_1(x) = 1$ for the determination of the the interpolating function $\epsilon(\lambda)$, yielded the ground state at energy = -0.479203. Here the aforementioned iterations were repeated until $\lambda = 1$ yielded a value to within 10^{-3}. When the Waxman algorithm was used to find the first excited state it did not yield a solution for $\lambda = 1$. Hence no spurious solutions were obtained with the algorithm. Only for $\lambda \geq 1.35348$ did the Gaussian potential support at least one excited bound state .

The spurious states arise in the case of the Lanczos algorithm because the resulting matrix representation of the Hamiltonian operator in the Lanczos basis corresponds to projecting it onto the space $\mathcal{F}$. The diagonalization of the resulting projected operator yields spurious eigenpairs. In the Waxman algorithm, iterations in each step are performed with the Hamiltonian operator and no projection or diagonalization is required. Hence, ultimately

only the exact bound states are obtained and there are no problems with spurious states.

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